



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:58 PM GMT

PDB ID : 4QJW  
Title : Crystal structure of catalytic domain of human carbonic anhydrase isozyme XII with inhibitor  
Authors : Smirnov, A.; Manakova, E.; Grazulis, S.  
Deposited on : 2014-06-05  
Resolution : 1.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

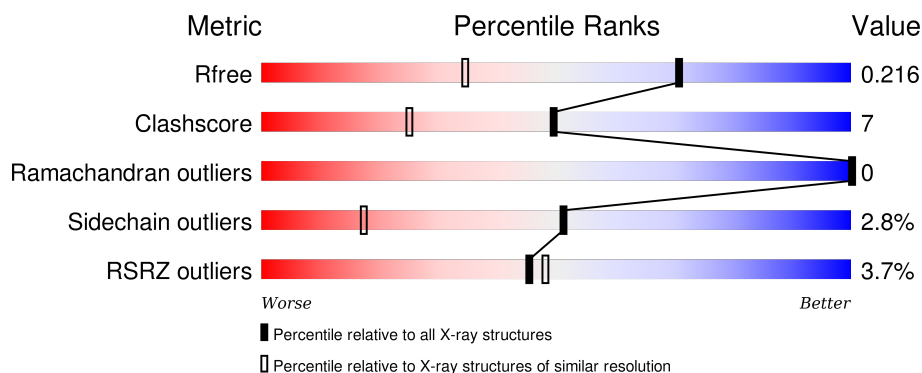
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1665 (1.58-1.54)
Clashscore	102246	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)
RSRZ outliers	91569	1668 (1.58-1.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	263	<div> <div>5%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	B	263	<div> <div>3%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>
1	C	263	<div> <div>4%</div> <div>86%</div> <div>13%</div> <div>..</div> </div>
1	D	263	<div> <div>3%</div> <div>86%</div> <div>13%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	WWO	A	302[A]	-	-	-	X
3	WWO	A	302[B]	-	-	-	X
3	WWO	B	302	-	-	X	X
3	WWO	C	302	-	-	-	X
3	WWO	D	302	-	-	-	X
4	EDO	D	304	-	-	X	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9883 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Carbonic anhydrase 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	3	0
			2121	1347	361	405	8			
1	B	261	Total	C	N	O	S	0	5	0
			2141	1357	366	410	8			
1	C	261	Total	C	N	O	S	0	4	0
			2123	1347	361	408	7			
1	D	261	Total	C	N	O	S	0	4	0
			2125	1350	361	407	7			

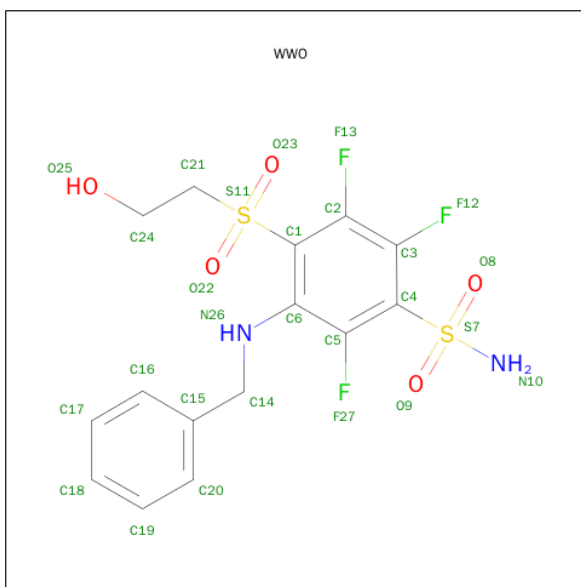
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP O43570
B	1	MET	-	EXPRESSION TAG	UNP O43570
C	1	MET	-	EXPRESSION TAG	UNP O43570
D	1	MET	-	EXPRESSION TAG	UNP O43570

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 3-(BENZYLAMINO)-2,5,6-TRIFLUORO-4-[(2-HYDROXYETHYL)SULFONYL]BENZENESULFONAMIDE (three-letter code: WWO) (formula: C<sub>15</sub>H<sub>15</sub>F<sub>3</sub>N<sub>2</sub>O<sub>5</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	1
			54	30	6	4	10	4		
3	B	1	Total	C	F	N	O	S	0	0
			27	15	3	2	5	2		
3	C	1	Total	C	F	N	O	S	0	0
			27	15	3	2	5	2		
3	D	1	Total	C	F	N	O	S	0	0
			27	15	3	2	5	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

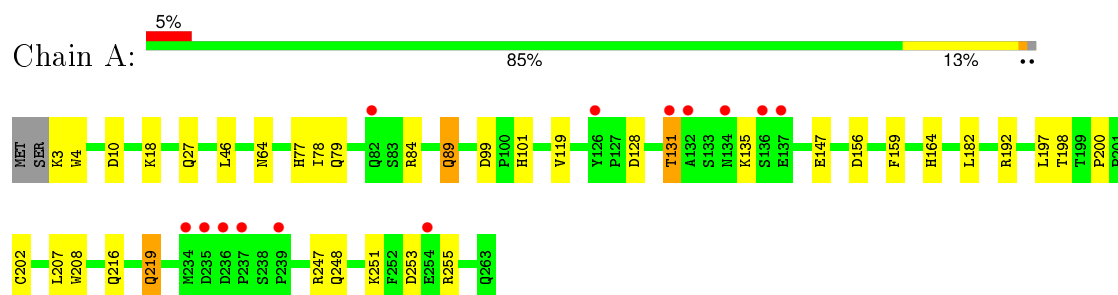
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	276	Total O 276 276	0	0
5	B	329	Total O 329 329	0	0
5	C	277	Total O 277 277	0	0
5	D	324	Total O 324 324	0	0

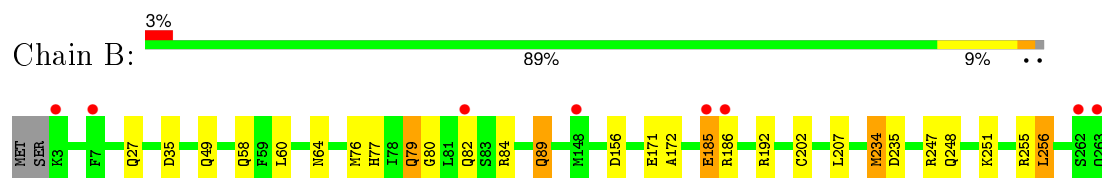
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

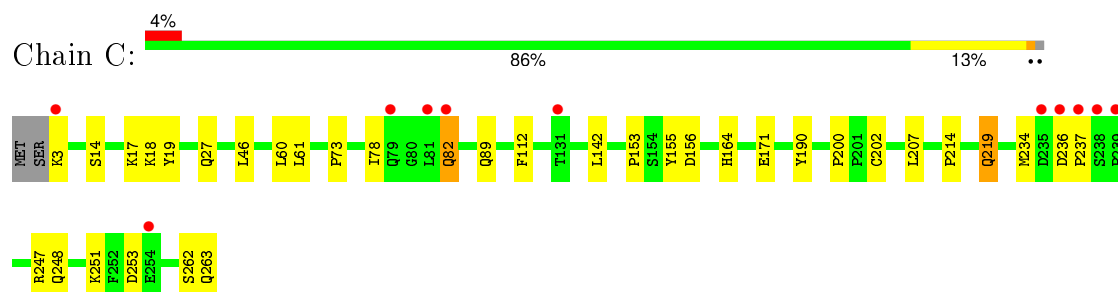
- Molecule 1: Carbonic anhydrase 12



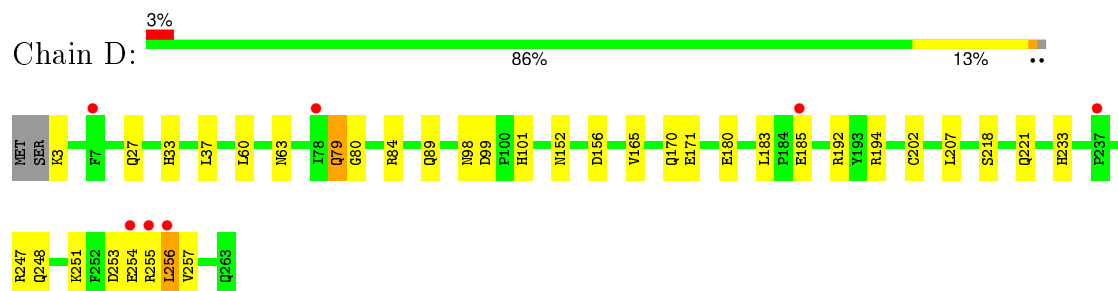
- Molecule 1: Carbonic anhydrase 12



- Molecule 1: Carbonic anhydrase 12



- Molecule 1: Carbonic anhydrase 12



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.50Å 66.76Å 80.47Å 81.57° 84.21° 86.66°	Depositor
Resolution (Å)	39.82 – 1.55 38.67 – 1.55	Depositor EDS
% Data completeness (in resolution range)	96.8 (39.82-1.55) 92.7 (38.67-1.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.185 , 0.222 0.179 , 0.216	Depositor DCC
$R_{free}$ test set	13154 reflections (10.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.4	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 50.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 133549 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9883	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.53 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.6995e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: WWO, ZN, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.09	1/2184 (0.0%)	1.11	5/2971 (0.2%)
1	B	1.10	0/2204	1.11	2/2998 (0.1%)
1	C	1.11	1/2187 (0.0%)	1.11	2/2977 (0.1%)
1	D	1.11	0/2188	1.10	2/2979 (0.1%)
All	All	1.10	2/8763 (0.0%)	1.10	11/11925 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	TRP	CD2-CE2	5.74	1.48	1.41
1	C	155	TYR	CG-CD1	5.52	1.46	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	LEU	CB-CG-CD1	5.97	121.16	111.00
1	A	255	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	219	GLN	CB-CG-CD	5.35	125.51	111.60
1	B	35	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	D	84	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	D	256	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	159	PHE	CB-CG-CD2	-5.13	117.21	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	C	142	LEU	CB-CG-CD1	-5.09	102.35	111.00
1	A	255	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	A	182	LEU	CB-CG-CD1	-5.00	102.50	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	262	SER	Mainchain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2121	0	2011	27	0
1	B	2141	0	2023	27	0
1	C	2123	0	2005	26	0
1	D	2125	0	2013	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	54	0	29	12	0
3	B	27	0	15	11	0
3	C	27	0	15	2	0
3	D	27	0	15	1	0
4	A	4	0	6	0	0
4	B	8	0	12	0	0
4	C	4	0	6	0	0
4	D	12	0	18	7	0
5	A	276	0	0	4	0
5	B	329	0	0	6	0
5	C	277	0	0	8	0
5	D	324	0	0	5	0
All	All	9883	0	8168	119	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ASN:HD21	3:B:302:WWO:H6	1.24	0.98
1:B:64:ASN:ND2	3:B:302:WWO:H6	1.83	0.94
1:B:64:ASN:HD21	3:B:302:WWO:C24	1.84	0.90
1:B:185:GLU:HG2	1:B:186:ARG:HH11	1.36	0.88
1:A:64:ASN:HD21	3:A:302[B]:WWO:H3	1.38	0.88
1:C:234:MET:CE	5:C:660:HOH:O	2.21	0.88
1:A:64:ASN:ND2	3:A:302[B]:WWO:H3	1.89	0.87
1:C:251:LYS:HZ2	1:D:248:GLN:HE21	1.22	0.84
1:D:192:ARG:HH21	4:D:304:EDO:C1	1.91	0.83
1:B:185:GLU:HG2	1:B:186:ARG:NH1	1.96	0.81
1:D:63:ASN:HB2	1:D:165[B]:VAL:HG12	1.64	0.79
1:D:218:SER:H	1:D:221:GLN:HE21	1.33	0.76
1:C:27:GLN:HE22	1:C:202:CYS:HB3	1.51	0.75
1:A:27:GLN:HE22	1:A:202:CYS:HB3	1.50	0.75
1:D:27:GLN:HE22	1:D:202:CYS:HB3	1.53	0.74
1:B:79:GLN:HG3	1:B:80:GLY:N	2.02	0.73
1:B:27:GLN:NE2	1:B:247:ARG:HH12	1.87	0.72
1:D:194:ARG:HD2	1:D:207:LEU:HD13	1.71	0.72
1:D:192:ARG:HH21	4:D:304:EDO:H12	1.57	0.69
1:B:64:ASN:HD22	3:B:302:WWO:H3	1.58	0.69
1:A:18[B]:LYS:HG3	1:A:18[B]:LYS:O	1.93	0.69
1:B:27:GLN:HE22	1:B:202:CYS:HB3	1.57	0.68
1:B:64:ASN:ND2	3:B:302:WWO:H3	2.09	0.68
1:D:63:ASN:CB	1:D:165[B]:VAL:HG12	2.24	0.68
1:D:152:ASN:H	1:D:221:GLN:HE22	1.42	0.67
1:A:27:GLN:NE2	1:A:247:ARG:HH12	1.92	0.66
1:C:234:MET:HE1	5:C:660:HOH:O	1.88	0.66
1:C:14[B]:SER:HB2	1:C:17:LYS:HE3	1.78	0.65
1:B:64:ASN:ND2	3:B:302:WWO:C24	2.51	0.65
1:A:89:GLN:HE22	3:A:302[B]:WWO:C24	2.09	0.64
1:C:27:GLN:NE2	1:C:247:ARG:HH12	1.96	0.64
1:A:99:ASP:OD1	1:A:101:HIS:HD2	1.82	0.62
1:A:251:LYS:HZ2	1:B:248:GLN:HE21	1.46	0.62
1:B:27:GLN:HE21	1:B:247:ARG:HH12	1.46	0.61
1:A:198:THR:OG1	3:A:302[A]:WWO:N10	2.34	0.61
1:C:46:LEU:HD22	1:C:78:ILE:CG2	2.31	0.61
1:D:27:GLN:NE2	1:D:247:ARG:HH12	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LYS:NZ	1:B:248:GLN:HE21	1.98	0.61
1:C:219:GLN:NE2	5:C:653:HOH:O	2.34	0.60
1:D:165[B]:VAL:HG13	1:D:170:GLN:O	2.02	0.60
1:C:248:GLN:HE21	1:D:251:LYS:HZ2	1.49	0.59
3:A:302[B]:WWO:F27	3:A:302[B]:WWO:C14	2.40	0.59
1:B:58:GLN:NE2	5:B:700:HOH:O	2.34	0.59
1:A:89:GLN:HE22	3:A:302[B]:WWO:H6	1.68	0.59
1:C:18:LYS:HD3	5:C:609:HOH:O	2.02	0.58
3:C:302:WWO:C14	3:C:302:WWO:F27	2.40	0.57
1:D:152:ASN:H	1:D:221:GLN:NE2	2.02	0.57
1:A:164:HIS:HD2	5:A:612:HOH:O	1.88	0.57
1:D:192:ARG:HG2	4:D:304:EDO:H12	1.86	0.57
1:A:27:GLN:HE21	1:A:247:ARG:HH12	1.52	0.57
1:B:64:ASN:ND2	3:B:302:WWO:C21	2.67	0.56
1:C:112:PHE:CE2	1:C:214[B]:PRO:HG2	2.40	0.56
1:A:3:LYS:NZ	5:A:664:HOH:O	2.25	0.56
1:B:185:GLU:HB2	5:B:651:HOH:O	2.06	0.55
1:C:60:LEU:HD11	1:C:171:GLU:HB3	1.88	0.54
1:C:164:HIS:HD2	5:C:560:HOH:O	1.89	0.54
1:D:3:LYS:N	5:D:724:HOH:O	2.40	0.53
1:C:234:MET:HE3	5:C:660:HOH:O	1.98	0.52
1:C:27:GLN:HE21	1:C:247:ARG:HH12	1.55	0.52
1:B:89:GLN:NE2	3:B:302:WWO:H4	2.24	0.52
1:D:255:ARG:NH2	5:D:442:HOH:O	2.29	0.52
3:A:302[B]:WWO:F27	3:A:302[B]:WWO:H9	1.99	0.51
1:A:79:GLN:NE2	1:A:84:ARG:HE	2.07	0.51
1:C:14[B]:SER:CB	1:C:17:LYS:HE3	2.40	0.51
1:B:84:ARG:HD2	5:B:575:HOH:O	2.11	0.51
1:D:79:GLN:HG3	1:D:80:GLY:N	2.25	0.51
1:D:180:GLU:HG3	1:D:183:LEU:HD12	1.93	0.50
1:A:198:THR:OG1	3:A:302[B]:WWO:N10	2.45	0.50
1:D:60:LEU:HD11	1:D:171:GLU:HB3	1.93	0.50
1:A:192:ARG:HD2	1:A:207:LEU:HD11	1.95	0.49
1:B:60:LEU:HD11	1:B:171:GLU:HB3	1.95	0.49
1:D:165[B]:VAL:HG12	1:D:165[B]:VAL:O	2.13	0.49
1:D:63:ASN:N	1:D:165[B]:VAL:HG11	2.29	0.47
1:D:27:GLN:HE21	1:D:247:ARG:HH12	1.63	0.47
1:C:253:ASP:OD1	5:C:552:HOH:O	2.20	0.47
1:C:27:GLN:HE21	1:C:247:ARG:HH22	1.63	0.47
1:A:77:HIS:ND1	5:A:574:HOH:O	2.34	0.47
3:D:302:WWO:F12	3:D:302:WWO:N10	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:ARG:HD2	1:B:207:LEU:HD11	1.97	0.46
1:D:98:ASN:CG	5:D:574:HOH:O	2.53	0.46
1:C:251:LYS:NZ	1:D:248:GLN:HE21	2.02	0.46
3:B:302:WWO:H3	5:B:604:HOH:O	2.16	0.46
1:D:192:ARG:HD2	4:D:304:EDO:H11	1.97	0.46
1:A:248:GLN:HE21	1:B:251:LYS:NZ	2.14	0.46
1:A:3:LYS:NZ	1:A:10:ASP:OD2	2.48	0.46
1:A:253:ASP:OD2	5:A:507:HOH:O	2.21	0.45
1:B:185:GLU:O	1:B:186:ARG:C	2.52	0.45
1:A:147:GLU:HG3	1:A:216:GLN:HG2	1.97	0.45
1:B:49:GLN:OE1	1:B:77:HIS:NE2	2.50	0.45
1:A:46:LEU:HD22	1:A:78:ILE:CG2	2.46	0.45
1:D:192:ARG:NH2	4:D:304:EDO:C1	2.71	0.44
1:B:234[A]:MET:HB3	1:B:234[A]:MET:HE3	1.65	0.44
3:A:302[A]:WWO:O22	3:A:302[A]:WWO:N26	2.49	0.44
1:D:33:HIS:HE1	5:D:495:HOH:O	2.00	0.44
1:A:197:LEU:HD22	3:A:302[A]:WWO:F27	2.08	0.43
1:D:253:ASP:O	1:D:254:GLU:HB2	2.18	0.43
1:D:192:ARG:NH2	4:D:304:EDO:O1	2.52	0.43
1:B:172:ALA:HB1	5:B:697:HOH:O	2.19	0.43
3:B:302:WWO:F27	3:B:302:WWO:C14	2.56	0.43
3:A:302[B]:WWO:F12	3:A:302[B]:WWO:N10	2.40	0.42
1:C:236:ASP:HA	1:C:237:PRO:HD3	1.84	0.42
1:C:263:GLN:NE2	5:C:669:HOH:O	2.51	0.42
3:C:302:WWO:H10	3:C:302:WWO:F27	2.07	0.42
1:C:19:TYR:CD1	1:C:200:PRO:HB3	2.55	0.42
3:B:302:WWO:H5	3:B:302:WWO:F13	2.10	0.41
1:C:61:LEU:O	1:C:171:GLU:HA	2.20	0.41
1:D:37:LEU:HD23	1:D:257:VAL:HB	2.00	0.41
1:B:255[A]:ARG:NH1	5:B:434:HOH:O	2.52	0.41
1:D:27:GLN:HE21	1:D:247:ARG:HH22	1.68	0.41
1:D:194:ARG:HD2	1:D:207:LEU:CD1	2.46	0.41
1:C:82:GLN:HE21	1:C:82:GLN:HB2	1.73	0.41
1:A:4:TRP:CG	1:A:200:PRO:HG2	2.56	0.41
1:A:128:ASP:OD1	1:A:131:THR:HG23	2.21	0.41
1:C:207:LEU:HA	1:C:207:LEU:HD12	1.90	0.41
1:A:119:VAL:HG11	3:A:302[A]:WWO:H10	2.02	0.40
1:D:192:ARG:HD2	4:D:304:EDO:C1	2.51	0.40
1:D:233:HIS:HE1	5:D:627:HOH:O	2.03	0.40
1:C:46:LEU:HD22	1:C:78:ILE:HG21	2.02	0.40
1:D:99:ASP:OD1	1:D:101:HIS:HD2	2.05	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/263 (100%)	254 (97%)	8 (3%)	0	100	100
1	B	264/263 (100%)	260 (98%)	4 (2%)	0	100	100
1	C	263/263 (100%)	259 (98%)	4 (2%)	0	100	100
1	D	263/263 (100%)	256 (97%)	7 (3%)	0	100	100
All	All	1052/1052 (100%)	1029 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/235 (100%)	231 (98%)	5 (2%)	61	29
1	B	238/235 (101%)	227 (95%)	11 (5%)	33	5
1	C	237/235 (101%)	230 (97%)	7 (3%)	48	15
1	D	237/235 (101%)	232 (98%)	5 (2%)	61	29
All	All	948/940 (101%)	920 (97%)	28 (3%)	51	15

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	131	THR
1	A	135	LYS
1	A	156	ASP
1	A	219	GLN
1	B	76	MET
1	B	79	GLN
1	B	82[A]	GLN
1	B	82[B]	GLN
1	B	89	GLN
1	B	156	ASP
1	B	185	GLU
1	B	234[A]	MET
1	B	234[B]	MET
1	B	235	ASP
1	B	256	LEU
1	C	3	LYS
1	C	73	PRO
1	C	82	GLN
1	C	89	GLN
1	C	153	PRO
1	C	156	ASP
1	C	219	GLN
1	D	79	GLN
1	D	89	GLN
1	D	156	ASP
1	D	185	GLU
1	D	256	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	49	GLN
1	A	79	GLN
1	A	101	HIS
1	A	111	HIS
1	A	164	HIS
1	A	248	GLN
1	B	27	GLN
1	B	56	ASN
1	B	58	GLN
1	B	111	HIS

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Mol	Chain	Res	Type
1	B	203	ASN
1	B	248	GLN
1	C	27	GLN
1	C	164	HIS
1	C	219	GLN
1	C	248	GLN
1	C	263	GLN
1	D	27	GLN
1	D	82	GLN
1	D	221	GLN
1	D	233	HIS
1	D	248	GLN
1	D	263	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	WWO	A	302[A]	2	26,28,28	2.90	5 (19%)	35,42,42	3.81	6 (17%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	WWO	A	302[B]	2	26,28,28	1.98	4 (15%)	35,42,42	4.06	18 (51%)
4	EDO	A	303	-	3,3,3	0.48	0	2,2,2	0.76	0
3	WWO	B	302	2	26,28,28	2.69	7 (26%)	35,42,42	2.74	12 (34%)
4	EDO	B	303	-	3,3,3	0.74	0	2,2,2	0.43	0
4	EDO	B	304	-	3,3,3	0.60	0	2,2,2	0.40	0
3	WWO	C	302	2	26,28,28	2.59	9 (34%)	35,42,42	3.67	16 (45%)
4	EDO	C	303	-	3,3,3	0.80	0	2,2,2	0.14	0
3	WWO	D	302	2	26,28,28	2.69	8 (30%)	35,42,42	3.79	11 (31%)
4	EDO	D	303	-	3,3,3	0.43	0	2,2,2	0.11	0
4	EDO	D	304	-	3,3,3	0.48	0	2,2,2	0.77	0
4	EDO	D	305	-	3,3,3	0.56	0	2,2,2	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	WWO	A	302[A]	2	-	0/21/21/21	0/2/2/2
3	WWO	A	302[B]	2	-	0/21/21/21	0/2/2/2
4	EDO	A	303	-	-	0/1/1/1	0/0/0/0
3	WWO	B	302	2	-	0/21/21/21	0/2/2/2
4	EDO	B	303	-	-	0/1/1/1	0/0/0/0
4	EDO	B	304	-	-	0/1/1/1	0/0/0/0
3	WWO	C	302	2	-	0/21/21/21	0/2/2/2
4	EDO	C	303	-	-	0/1/1/1	0/0/0/0
3	WWO	D	302	2	-	0/21/21/21	0/2/2/2
4	EDO	D	303	-	-	0/1/1/1	0/0/0/0
4	EDO	D	304	-	-	0/1/1/1	0/0/0/0
4	EDO	D	305	-	-	0/1/1/1	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302[B]	WWO	F27-C5	-3.01	1.30	1.35
3	C	302	WWO	C3-C4	2.06	1.42	1.39
3	B	302	WWO	C4-S7	2.14	1.83	1.79
3	B	302	WWO	C6-C1	2.38	1.43	1.40
3	D	302	WWO	C2-C1	2.55	1.42	1.39
3	B	302	WWO	O9-S7	2.64	1.48	1.43
3	D	302	WWO	O9-S7	2.68	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	WWO	O9-S7	2.70	1.48	1.43
3	C	302	WWO	F13-C2	2.75	1.39	1.35
3	D	302	WWO	C6-C1	2.93	1.43	1.40
3	C	302	WWO	C4-S7	3.01	1.84	1.79
3	A	302[B]	WWO	O23-S11	3.26	1.49	1.44
3	C	302	WWO	S7-N10	3.29	1.67	1.60
3	C	302	WWO	O8-S7	3.41	1.49	1.43
3	D	302	WWO	C21-S11	3.43	1.85	1.78
3	C	302	WWO	C6-C1	3.93	1.44	1.40
3	D	302	WWO	S7-N10	4.41	1.70	1.60
3	A	302[B]	WWO	S7-N10	4.57	1.70	1.60
3	B	302	WWO	O8-S7	5.38	1.53	1.43
3	D	302	WWO	O8-S7	5.55	1.53	1.43
3	D	302	WWO	O23-S11	5.77	1.53	1.44
3	A	302[A]	WWO	O23-S11	5.93	1.54	1.44
3	A	302[A]	WWO	O22-S11	5.94	1.54	1.44
3	A	302[A]	WWO	O8-S7	5.97	1.54	1.43
3	A	302[A]	WWO	O9-S7	6.06	1.54	1.43
3	B	302	WWO	O23-S11	6.07	1.54	1.44
3	B	302	WWO	S7-N10	6.30	1.74	1.60
3	C	302	WWO	O22-S11	6.33	1.54	1.44
3	A	302[B]	WWO	O22-S11	6.47	1.55	1.44
3	C	302	WWO	O23-S11	6.60	1.55	1.44
3	D	302	WWO	O22-S11	6.71	1.55	1.44
3	B	302	WWO	O22-S11	6.93	1.55	1.44
3	A	302[A]	WWO	S7-N10	7.41	1.76	1.60

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	WWO	O22-S11-O23	-17.82	94.85	118.40
3	A	302[A]	WWO	O22-S11-O23	-15.10	98.44	118.40
3	A	302[B]	WWO	O22-S11-O23	-12.19	102.30	118.40
3	C	302	WWO	O22-S11-O23	-12.00	102.54	118.40
3	A	302[A]	WWO	O8-S7-O9	-11.96	101.99	118.80
3	B	302	WWO	O22-S11-O23	-10.65	104.32	118.40
3	A	302[B]	WWO	O8-S7-O9	-10.30	104.32	118.80
3	C	302	WWO	O8-S7-O9	-6.09	110.25	118.80
3	B	302	WWO	C15-C14-N26	-5.74	100.42	113.73
3	C	302	WWO	C15-C14-N26	-5.45	101.09	113.73
3	C	302	WWO	C4-S7-N10	-5.12	99.54	108.38
3	A	302[B]	WWO	O8-S7-N10	-5.01	100.79	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	WWO	C15-C14-N26	-4.69	102.86	113.73
3	A	302[B]	WWO	C3-C2-C1	-4.67	116.23	121.66
3	D	302	WWO	C4-S7-N10	-3.88	101.68	108.38
3	A	302[B]	WWO	O25-C24-C21	-3.86	102.31	109.98
3	B	302	WWO	C4-S7-N10	-3.76	101.87	108.38
3	C	302	WWO	O23-S11-C21	-3.46	103.71	108.08
3	A	302[B]	WWO	C4-S7-N10	-3.35	102.59	108.38
3	B	302	WWO	O9-S7-C4	-3.08	102.83	107.31
3	C	302	WWO	F27-C5-C4	-2.99	116.25	120.97
3	C	302	WWO	F12-C3-C2	-2.83	113.25	119.28
3	A	302[B]	WWO	F27-C5-C4	-2.62	116.83	120.97
3	C	302	WWO	O22-S11-C21	-2.57	104.83	108.08
3	C	302	WWO	C5-C6-N26	-2.53	114.84	122.55
3	B	302	WWO	F27-C5-C4	-2.49	117.05	120.97
3	D	302	WWO	F27-C5-C4	-2.46	117.09	120.97
3	D	302	WWO	C6-C1-C2	-2.45	116.45	120.03
3	D	302	WWO	C5-C6-N26	-2.41	115.19	122.55
3	A	302[B]	WWO	C6-C5-C4	-2.36	117.74	121.75
3	B	302	WWO	F12-C3-C2	-2.34	114.30	119.28
3	A	302[B]	WWO	F12-C3-C2	-2.28	114.43	119.28
3	A	302[B]	WWO	O23-S11-C1	-2.11	100.63	106.45
3	A	302[B]	WWO	C5-C6-N26	-2.02	116.38	122.55
3	B	302	WWO	O9-S7-N10	2.03	109.91	107.28
3	B	302	WWO	C14-N26-C6	2.09	125.25	116.08
3	C	302	WWO	C2-C3-C4	2.15	124.17	121.66
3	C	302	WWO	F13-C2-C1	2.16	124.40	120.97
3	B	302	WWO	C20-C15-C16	2.19	121.64	118.13
3	C	302	WWO	O22-S11-C1	2.23	112.59	106.45
3	A	302[B]	WWO	O22-S11-C1	2.23	112.61	106.45
3	B	302	WWO	O25-C24-C21	2.26	114.48	109.98
3	D	302	WWO	O8-S7-C4	2.45	110.87	107.31
3	C	302	WWO	C20-C15-C16	2.55	122.22	118.13
3	C	302	WWO	O9-S7-N10	2.72	110.80	107.28
3	D	302	WWO	O22-S11-C1	2.91	114.49	106.45
3	A	302[B]	WWO	C5-C6-C1	3.17	121.24	116.30
3	A	302[A]	WWO	O8-S7-C4	3.61	112.55	107.31
3	B	302	WWO	C21-S11-C1	3.87	117.12	105.83
3	D	302	WWO	O8-S7-N10	3.96	112.41	107.28
3	A	302[B]	WWO	O9-S7-C4	3.99	113.11	107.31
3	A	302[B]	WWO	F27-C5-C6	4.17	125.38	119.56
3	D	302	WWO	C21-S11-C1	4.39	118.62	105.83
3	B	302	WWO	O8-S7-N10	4.57	113.20	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302[A]	WWO	O9-S7-C4	4.76	114.23	107.31
3	A	302[A]	WWO	C4-S7-N10	4.92	116.88	108.38
3	C	302	WWO	C21-S11-C1	5.01	120.45	105.83
3	A	302[B]	WWO	C21-S11-C1	5.58	122.09	105.83
3	A	302[B]	WWO	O9-S7-N10	6.23	115.35	107.28
3	D	302	WWO	O25-C24-C21	6.46	122.81	109.98
3	A	302[A]	WWO	C21-S11-C1	7.02	126.31	105.83
3	A	302[B]	WWO	O8-S7-C4	9.11	120.54	107.31
3	C	302	WWO	O8-S7-C4	10.52	122.59	107.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302[A]	WWO	4	0
3	A	302[B]	WWO	8	0
3	B	302	WWO	11	0
3	C	302	WWO	2	0
3	D	302	WWO	1	0
4	D	304	EDO	7	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	261/263 (99%)	0.45	13 (4%) 32 33	6, 13, 29, 47	1 (0%)
1	B	261/263 (99%)	0.40	8 (3%) 52 56	6, 13, 25, 41	0
1	C	261/263 (99%)	0.36	11 (4%) 40 41	6, 12, 26, 60	1 (0%)
1	D	261/263 (99%)	0.35	7 (2%) 58 62	5, 12, 24, 50	1 (0%)
All	All	1044/1052 (99%)	0.39	39 (3%) 45 48	5, 13, 26, 60	3 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	ASP	6.5
1	C	237	PRO	6.1
1	B	185	GLU	4.8
1	C	235	ASP	4.8
1	C	238	SER	4.4
1	A	131	THR	4.3
1	A	237	PRO	4.2
1	A	254	GLU	4.1
1	A	239	PRO	3.9
1	C	82	GLN	3.4
1	A	136	SER	3.3
1	B	262	SER	3.3
1	B	263	GLN	3.2
1	C	254	GLU	3.1
1	C	81	LEU	3.0
1	B	82[A]	GLN	2.9
1	D	185	GLU	2.7
1	D	237	PRO	2.6
1	A	82	GLN	2.5
1	B	186	ARG	2.5
1	A	134	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	148	MET	2.5
1	D	254	GLU	2.5
1	C	236	ASP	2.4
1	B	3	LYS	2.4
1	C	3	LYS	2.4
1	C	239	PRO	2.3
1	A	236	ASP	2.3
1	A	132	ALA	2.2
1	D	256	LEU	2.2
1	C	79	GLN	2.2
1	A	234[A]	MET	2.2
1	B	7	PHE	2.2
1	D	7	PHE	2.1
1	A	126	TYR	2.1
1	A	137	GLU	2.1
1	D	78[A]	ILE	2.0
1	D	255	ARG	2.0
1	C	131	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	WWO	A	302[A]	27/27	0.86	0.23	7.16	13,25,33,34	27
3	WWO	A	302[B]	27/27	0.86	0.23	7.04	13,22,28,29	27
3	WWO	C	302	27/27	0.90	0.19	5.54	14,29,39,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	D	304	4/4	0.79	0.20	4.40	28,32,33,38	0
3	WWO	D	302	27/27	0.94	0.14	3.48	13,24,34,41	0
3	WWO	B	302	27/27	0.91	0.16	2.57	12,27,40,51	0
4	EDO	B	304	4/4	0.86	0.12	0.10	21,22,22,24	0
2	ZN	B	301	1/1	1.00	0.09	-0.22	8,8,8,8	0
4	EDO	D	303	4/4	0.88	0.10	-0.25	24,28,32,33	0
4	EDO	C	303	4/4	0.92	0.09	-0.49	19,23,26,27	0
2	ZN	D	301	1/1	1.00	0.08	-0.80	7,7,7,7	0
4	EDO	B	303	4/4	0.92	0.09	-0.83	14,15,16,16	0
4	EDO	A	303	4/4	0.95	0.09	-1.97	18,23,24,25	0
2	ZN	C	301	1/1	1.00	0.08	-	7,7,7,7	0
4	EDO	D	305	4/4	0.65	0.22	-	46,51,53,62	0
2	ZN	A	301	1/1	1.00	0.09	-	7,7,7,7	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.